

=> E "2,3,5-TRIMETHYLHYDROQUINONE"/CN 25

E1	1	2,3,5-TRIMETHYLHEXANONITRILE/CN
E2	1	2,3,5-TRIMETHYLHEXENE/CN
E3	1 -->	2,3,5-TRIMETHYLHYDROQUINONE/CN
E4	1	2,3,5-TRIMETHYLHYDROQUINONE DIACETATE/CN
E5	1	2,3,5-TRIMETHYLHYDROQUINONE DIPHOSPHATE TETRASODIUM SALT/CN
E6	1	2,3,5-TRIMETHYLINDOLE/CN
E7	1	2,3,5-TRIMETHYLINDOLYL 3-HYDROPEROXIDE/CN
E8	1	2,3,5-TRIMETHYLISOTHIAZOLIUM CATION/CN
E9	1	2,3,5-TRIMETHYLISOTHIAZOLIUM PERCHLORATE/CN
E10	1	2,3,5-TRIMETHYLISOXAZOLIUM IODIDE/CN
E11	1	2,3,5-TRIMETHYLNAPHTHALENE/CN
E12	1	2,3,5-TRIMETHYLNITROBENZENE/CN
E13	1	2,3,5-TRIMETHYLNONANOIC ACID/CN
E14	1	2,3,5-TRIMETHYLOXAZOLIUM IODIDE/CN
E15	1	2,3,5-TRIMETHYLPENTADECANOIC ACID/CN
E16	1	2,3,5-TRIMETHYLPHENANTHRENE/CN
E17	1	2,3,5-TRIMETHYLPHENOL/CN
E18	1	2,3,5-TRIMETHYLPHENOL FORMATE/CN
E19	1	2,3,5-TRIMETHYLPHENOL SODIUM SALT/CN
E20	1	2,3,5-TRIMETHYLPHENOXYACETAMIDE/CN
E21	1	2,3,5-TRIMETHYLPHENYL 1,2-NAPHTHOQUINONE
DIAZIDE-(2)-5-SULFONATE/CN		
E22	1	2,3,5-TRIMETHYLPHENYL 2,4,5-TRIMETHYLPHENYL SULFONE/CN
E23	1	2,3,5-TRIMETHYLPHENYL ACETATE/CN
E24	1	2,3,5-TRIMETHYLPHENYL ACETIC ACID/CN
E25	1	2,3,5-TRIMETHYLPHENYL BENZYL ETHER/CN

=> S E3

L1 1 "2,3,5-TRIMETHYLHYDROQUINONE"/CN

=> D L1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 700-13-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN 1,4-Benzenediol, 2,3,5-trimethyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Hydroquinone, trimethyl- (6CI, 7CI, 8CI)

OTHER NAMES:

CN  $\psi$ -Cumohydroquinone

CN 1,4-Dihydroxy-2,3,5-trimethylbenzene

CN 2,3,5-Trimethyl-1,4-benzenediol

CN 2,3,5-Trimethyl-1,4-hydroquinone

CN 2,3,5-Trimethyl-p-hydroquinone

CN 2,3,5-Trimethylhydroquinone

CN NSC 401617

CN Pseudocumohydroquinone

CN Trimethyl-p-hydroquinone

CN Trimethylhydroquinone

MF C9 H12 O2

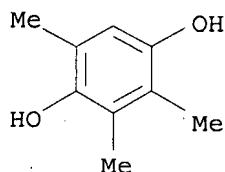
CI COM

LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PROMT, PS, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

923 REFERENCES IN FILE CA (1907 TO DATE)  
 6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 925 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 31 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> E "2,3,5-TRIMETHYLHYDROQUINONE DIALKONATE"/CN 25

E1	1	2,3,5-TRIMETHYLHYDROQUINONE/CN
E2	1	2,3,5-TRIMETHYLHYDROQUINONE DIACETATE/CN
E3	0 -->	2,3,5-TRIMETHYLHYDROQUINONE DIALKONATE/CN
E4	1	2,3,5-TRIMETHYLHYDROQUINONE DIPHOSPHATE TETRASODIUM SALT/CN
E5	1	2,3,5-TRIMETHYLINDOLE/CN
E6	1	2,3,5-TRIMETHYLINDOLYL 3-HYDROPEROXIDE/CN
E7	1	2,3,5-TRIMETHYLISOTHIAZOLIUM CATION/CN
E8	1	2,3,5-TRIMETHYLISOTHIAZOLIUM PERCHLORATE/CN
E9	1	2,3,5-TRIMETHYLISOXAZOLIUM IODIDE/CN
E10	1	2,3,5-TRIMETHYLNAPHTHALENE/CN
E11	1	2,3,5-TRIMETHYLNITROBENZENE/CN
E12	1	2,3,5-TRIMETHYLNONANOIC ACID/CN
E13	1	2,3,5-TRIMETHYLOXAZOLIUM IODIDE/CN
E14	1	2,3,5-TRIMETHYLPENTADECANOIC ACID/CN
E15	1	2,3,5-TRIMETHYLPHENANTHRENE/CN
E16	1	2,3,5-TRIMETHYLPHENOL/CN
E17	1	2,3,5-TRIMETHYLPHENOL FORMATE/CN
E18	1	2,3,5-TRIMETHYLPHENOL SODIUM SALT/CN
E19	1	2,3,5-TRIMETHYLPHENOXYACETAMIDE/CN
E20	1	2,3,5-TRIMETHYLPHENYL 1,2-NAPHTHOQUINONE
DIAZIDE-(2)-5-SULFONATE/CN		
E21	1	2,3,5-TRIMETHYLPHENYL 2,4,5-TRIMETHYLPHENYL SULFONE/CN
E22	1	2,3,5-TRIMETHYLPHENYL ACETATE/CN
E23	1	2,3,5-TRIMETHYLPHENYL ACETIC ACID/CN
E24	1	2,3,5-TRIMETHYLPHENYL BENZYL ETHER/CN
E25	1	2,3,5-TRIMETHYLPHENYL METHYLCARBAMATE/CN

=> E "2,3,5-TRIMETHYLHYDROQUINONE DIMETHONATE"/CN 25

E1	1	2,3,5-TRIMETHYLHYDROQUINONE/CN
E2	1	2,3,5-TRIMETHYLHYDROQUINONE DIACETATE/CN
E3	0 -->	2,3,5-TRIMETHYLHYDROQUINONE DIMETHONATE/CN
E4	1	2,3,5-TRIMETHYLHYDROQUINONE DIPHOSPHATE TETRASODIUM SALT/CN
E5	1	2,3,5-TRIMETHYLINDOLE/CN
E6	1	2,3,5-TRIMETHYLINDOLYL 3-HYDROPEROXIDE/CN
E7	1	2,3,5-TRIMETHYLISOTHIAZOLIUM CATION/CN
E8	1	2,3,5-TRIMETHYLISOTHIAZOLIUM PERCHLORATE/CN
E9	1	2,3,5-TRIMETHYLISOXAZOLIUM IODIDE/CN
E10	1	2,3,5-TRIMETHYLNAPHTHALENE/CN
E11	1	2,3,5-TRIMETHYLNITROBENZENE/CN
E12	1	2,3,5-TRIMETHYLNONANOIC ACID/CN
E13	1	2,3,5-TRIMETHYLOXAZOLIUM IODIDE/CN
E14	1	2,3,5-TRIMETHYLPENTADECANOIC ACID/CN
E15	1	2,3,5-TRIMETHYLPHENANTHRENE/CN
E16	1	2,3,5-TRIMETHYLPHENOL/CN
E17	1	2,3,5-TRIMETHYLPHENOL FORMATE/CN
E18	1	2,3,5-TRIMETHYLPHENOL SODIUM SALT/CN

E19	1	2,3,5-TRIMETHYLPHENOXYACETAMIDE/CN
E20	1	2,3,5-TRIMETHYLPHENYL 1,2-NAPHTHOQUINONE
DIAZIDE-(2)-5-SULFONATE/CN		
E21	1	2,3,5-TRIMETHYLPHENYL 2,4,5-TRIMETHYLPHENYL SULFONE/CN
E22	1	2,3,5-TRIMETHYLPHENYL ACETATE/CN
E23	1	2,3,5-TRIMETHYLPHENYL ACETIC ACID/CN
E24	1	2,3,5-TRIMETHYLPHENYL BENZYL ETHER/CN
E25	1	2,3,5-TRIMETHYLPHENYL METHYL CARBAMATE/CN

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

9.15

9.36

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FILE LAST UPDATED: 10 Jul 2007 (20070710/ED)

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=> S L1

L2 925 L1

=> S ALKONATE

3 ALKONATE

2 ALKONATES

L3 5 ALKONATE

(ALKONATE OR ALKONATES)

=> S DIALKONATE

L4 1 DIALKONATE

=> S KETOISOPHORONE

81 KETOISOPHORONE

1 KETOISOPHORONES

L5 82 KETOISOPHORONE

(KETOISOPHORONE OR KETOISOPHORONES)

=> S L2 AND L5

L6 3 L2 AND L5

=> D BIB ABS HITSTR

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:570864 CAPLUS

DN 143:77878

TI Catalytic esterification process for the manufacture of  
trimethylhydroquinone dialkanoates  
IN Bonrath, Werner; Foricher, Yann  
PA DSM IP Assets B. V., Neth.  
SO PCT Int. Appl., 12 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005058792	A1	20050630	WO 2004-EP13903	20041207
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1694628	A1	20060830	EP 2004-803588	20041207
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
	CN 1886361	A	20061227	CN 2004-80035561	20041207
	JP 2007516262	T	20070621	JP 2006-544280	20041207
	US 2007049762	A1	20070301	US 2006-582672	20060629
PRAI	EP 2003-28811	A	20031215		
	WO 2004-EP13903	W	20041207		

OS CASREACT 143:77878

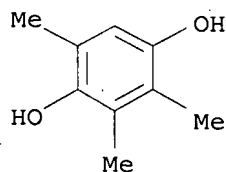
AB A process for the manufacture of a 2,3,5-trimethylhydroquinone dialkanoate comprises reacting ketoisophorone with an acylating agent in the presence of an indium salt as the catalyst. Preferred are indium(III) salts such as indium trichloride or indium tris(trifluoromethanesulfonate). Process for the manufacture of 2,3,5-trimethylhydroquinone using 2,3,5-trimethylhydroquinone dialkanoate as the starting material, especially a process for the manufacture of 2,3,5-trimethylhydroquinone by transesterification of 2,3,5-trimethylhydroquinone dialkanoate, as well as a process for the manufacture of  $\alpha$ -tocopherol and its alkanates, especially

of (all-racemic)- $\alpha$ -tocopherol and its acetate, comprising the reaction of ketoisophorone to 2,3,5-trimethylhydroquinone dialkanoate are presented.

IT 700-13-0, 2,3,5-Trimethylhydroquinone  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(esterification of)

RN 700-13-0 CAPLUS

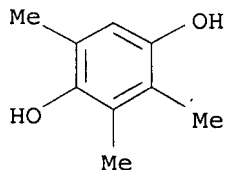
CN 1,4-Benzenediol, 2,3,5-trimethyl- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> D BIB ABS HITSTR 2-3

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2001:740313 CAPLUS  
DN 136:71494  
TI Industrial application of Nafion-systems in rearrangement-aromatisation, transesterification, alkylation, and ring-closure reactions  
AU Schneider, M.; Zimmermann, K.; Aquino, F.; Bonrath, W.  
CS Vitamins and Fine Chemicals Division, Chemical Process Technology, F. Hoffmann-La Roche Ltd., Basel, CH-4070, Switz.  
SO Applied Catalysis, A: General (2001), 220(1-2), 51-58  
CODEN: ACAGE4; ISSN: 0926-860X  
PB Elsevier Science B.V.  
DT Journal  
LA English  
AB Nafion, a perfluorinated sulfonic acid ion-exchange polymer, is known to be a very strong Bronsted acid. Thus, Nafion NR 50 and Nafion/SiO<sub>2</sub> with 15 weight % Nafion-loading were selected, in order to elucidate the potential for rearrangement-aromatization of ketoisophorone (KIP) to 2,3,5-trimethylhydroquinone diacetate (TMHQ-DA) in presence of acetic acid anhydride as acylating agent, transesterification of TMHQ-DA to 2,3,6-trimethylhydroquinone monoacetate (TMHQ-1-MA) and reaction of isophytol (IP) with trimethylhydroquinone (TMHQ) to (all-rac)- $\alpha$ -tocopherol. For the rearrangement-aromatization of KIP to TMHQ-DA supported Nafion/SiO<sub>2</sub> was markedly more active than the unsupported Nafion NR 50. Both Nafion-systems generally revealed remarkably high selectivity, which ranged up to 94 GC-a% TMHQ-DA at high conversion. The major side-product was 3,4,5-trimethylcatechol diacetate. In case of Nafion/SiO<sub>2</sub>, pre-treatment under vacuum and especially grinding of the extrudates seemed to increase activity at comparably high selectivity. Recycling Nafion/SiO<sub>2</sub> after filtering and rinsing with acetic acid anhydride led to gradually decreasing activity. Without intermediate isolation of TMHQ-DA, Nafion/SiO<sub>2</sub> was active and selective for the formation of TMHQ-1-MA. Using the Nafion systems in the reaction of IP and TMHQ revealed that remarkably high conversion of IP (>95%) and, compared with zinc chloride/Bronsted acid or BF<sub>3</sub>-catalyzed reaction good yields ( $\approx$ 92%) and selectivities were obtained. We found a strong dependency on the solvent polarity. In further expts., the recovery of the catalyst was tested.  
IT 700-13-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(Nafion-catalyzed preparation and cyclization reaction of trimethylhydroquinone with isophytol)  
RN 700-13-0 CAPLUS  
CN 1,4-Benzenediol, 2,3,5-trimethyl- (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2001:297544 CAPLUS  
DN 134:295967  
TI Process for the preparation of esters of chroman derivatives  
IN Weigel, Horst; Krill, Steffen; Hasselbach, Hans Joachim; Huthmacher, Klaus

PA Degussa-Huls A.-G., Germany  
 SO Eur. Pat. Appl., 14 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA German  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1094062	A1	20010425	EP 2000-116383	20000728
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	DE 19951006	A1	20010426	DE 1999-19951006	19991022
	IN 188710	A1	20021026	IN 2000-CA582	20001016
	CA 2323840	A1	20010422	CA 2000-2323840	20001019
	CN 1308077	A	20010815	CN 2000-129870	20001019
	US 6329535	B1	20011211	US 2000-692313	20001020
	IL 139178	A	20040725	IL 2000-139178	20001020
PRAI	DE 1999-19951006	A	19991022		

OS CASREACT 134:295967

AB Process for the preparation of chroman ester derivs., in that one, (1.1) reacts tech. pure ketoisophorone with a acylating agent in the presence of a protonic acid to give a trimethylhydroquinone ester, and (1.2) this ester is reacted with allyl alc. or its derivative in the presence of zinc halide and a proton cleaving acid, and (1.3) carried out in the presence of an organic solvent, is characterized by (1.1.1) the solution in reaction

step

(1.1) is cooled to a temperature between 5 and 40°, (1.1.2) the crystallized product is separated and washed, (1.1.3) that the saved filtrate from the separated product and the washes is out into the solvent for future reaction step (1.1), (1.2.1) the washed product without drying is introduced into reaction (1.2) and, (1.2.2) the desired product isolated after further acylation.. Thus, ketoisophorone is reacted with Ac2O in the presence of triflic acid, to give 87% trimethylhydroquinone diacetate; the latter is reacted with isophytol in PhMe containing ZnBr2 and HBr followed by Ac2O to give 95.6% vitamin E acetate.

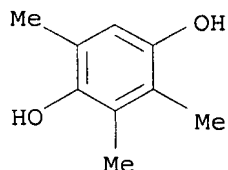
IT 700-13-0DP, Trimethylhydroquinone, esters

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of chroman ester derivs. via acylation of ketoisophorone followed by reaction with allyl alc. derivs.)

RN 700-13-0 CAPLUS

CN 1,4-Benzenediol, 2,3,5-trimethyl- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT